4,4'-(Propane-2,2-diyl)di($^{13}C_6$)phenol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 24.1

Global applicability domain: Inside

Local applicability domain index: 4.92e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

Image not found
Oxydisulfoton
Measured: 1.00
Predicted: 1.63

Image not found
Disulfoton
Measured: 219
Predicted: 151

Image not found
Parathion
Measured: 97.7
Predicted: 22.3

Image not found
O,O-Diethyl dithiophosphate
Measured: 5.01
Predicted: 5.43

Image not found
Methyl parathion
Measured: 85.1
Predicted: 14.5